

5-«alpha»-Androstan-3-«alpha»-ol-17-«beta»-carb

MeTMS

InChI: InChI=1S/C24H42O3Si/c1-23-13-11-17(27-28(4,5)6)15-16(23)7-8-18-19-9-10-21(22(25)26)3
InChIKey: WGNHKXCUYIUHGD-NXNBNPKKSA-N
Formula: C24H42O3Si
SMILES: COC(=O)C1CCC2C3CCC4CC(O[Si](C)(C)C)CCC4(C)C3CCC12C
Mol. weight [g/mol]: 406.67

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.87		Crippen Method
logp	6.038		Crippen Method
rinpol	2644.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R393289&Units=SI>

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
rinpol: Non-polar retention indices

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